

**SHAMSA BIBI**  
**PhD, Post Doc.**

**PROFILE**



DOB : 19 December 1985  
Nationality : Pakistan  
Material status : Married  
Languages : English, Chinese, Urdu, and Punjabi.  
Address : Current  
Chemistry Department,  
University of Agriculture Faisalabad (UAF)  
Contact : Cell Phone : +92 332 445 5210 (Pakistan)  
Email : shamsa.shafiq@uaf.edu.pk

**EDUCATION**



**PhD in Physical/Computational Chemistry**, Northeast Normal University, PR China 2010-2014  
Dissertation title: *Rational Design of the Highly Efficient Sulfur Containing Small Molecular Donor Materials for Organic Photovoltaic Cells.*  
(1 year Chinese Language 2010-2011)



**Master of Science in Chemistry**, University of the Punjab, Lahore, Pak Majors: Inorganic Chemistry 2006-2008



**Bachelor of Science**, University of the Punjab, Lahore Pak Majors: Chemistry / Biological Sciences 2004-2006

## WORK



**Postdoctoral  
Researcher**

Postdoctoral fellow, State Key Laboratory of  
Theoretical and Computational Chemistry, Institute of  
Theoretical Chemistry, Jilin University, PR China

2014-2015



**Assistant Professor**

Chemistry Department,  
University of Agriculture Faisalabad (UAF)

2015 to May 2024

**Associate Professor**

<https://web.uaf.edu.pk/FacultyProfile/Profile/55>

May 2024 to date

## SCHOLARSHIPS AND AWARDS

- Chinese Government Scholarship (PhD) 2010, Northeast Normal University, PR China
- Postdoctoral Fellowship 2014. State Key Laboratory of Theoretical and Computational Chemistry, Jilin University
- Government Merit scholarship for M.Sc. 2006, Punjab University Lahore, Pakistan.

## RESEARCH INTERESTS

**Using Machine Learning and Computational Tools**, Theoretical and Computational analysis for Materials including Organic Photovoltaics, Pharmaceutical Applications & pesticides for Agriculture applications

## COMPUTATIONAL SKILLS/ EXPERTISE SOFTWARE-HARDWARE:

Gaussian 09/16, Gauss view, Material Studio, Discovery Studio, Gauss Sum, Ultra Edit, Pymolyze, Multiwfn, Chema Draw, EndNote, Adobe Photoshop, Linux, Window OS, Molekel, Molden, Mercury, MATLAB

## CALCULATION SKILLS IN COMPUTATIONAL/THEORETICAL CHEMISTRY

- Molecular geometries calculations using Density Functional Theory (DFT) methods.
- Ground state optimization and frequency calculations.
- Molecular orbital calculations.
- Electronic properties calculations.
- Natural transition orbital (NTO) analysis calculations.
- Percentage contribution analysis by calculating total density of states (TDOS) and projected partial density of states (PDOS).
- Simulation of electronic absorption spectra by Time Dependent-DFT (TD-DFT) methods.
- Reorganization energy calculations in gaseous phase.
- Mobility calculations in the crystalline state structure.
- Generation of the electron density difference map (EDDM) of the transition states to understand the nature of the excited state.
- Potential energy surfaces to predict molecules stability.
- Non-Covalent interaction (NCI) analysis
- IR and NMR calculation analysis

## RESEARCH PROJECTS AND GRANTS

### A. Research Projects as PI Awarded

- i. **PI - Start-Up Research Grant Program “Establishment of Computational Chemistry Lab. at UAF” (~ 0.5 million PKR)** by Higher Education Commission Pakistan (Completed 2015-17)
- ii. **Awarded International funding for “Foreign Research Collaboration Project under “One Road One Belt” project Grant # DL20180036 (~ 37,000 USD) by Jilin University and Ministry of Education of People’s Republic of China**, with institute of Theoretical Chemistry, Jilin University, Changchun, China under, from November 23-30th, 2018-2019 (completed 2018-19).
- iii. **International Research collaboration Project by Deanship of Scientific Research, King Khalid University Ministry of Education, Kingdom of Saudia Arabia under project # RGP. 2/272/44 (~ 1.6 million PKR) 2024-26 (Awarded~ continue).**

### B. Research Projects as Team Scientist/ Co-PI Equivalent Awarded

1. Punjab Agriculture Research Board (PARB), Pakistan, Project # 20-419 of 7.794 million PKR by PARB (2021-24 Completed)

## COURSE TAUGHT TO:

Ph.D., M.Phil., M.Sc., Undergraduate, F.Sc Pre-Agriculture.

## STUDENTS UNDER SUPERVISION

|                                                            |   |                  |
|------------------------------------------------------------|---|------------------|
| <i>Ph.D. Students (As a Main Supervisor)</i>               | = | 03 (completed)   |
| <i>Ph.D. Students (As a Main Supervisor)</i>               | = | 03 (in progress) |
| <i>Ph.D. Students (As a Committee Member)</i>              | = | 01 (completed)   |
| Ph.D. Students (As a Committee Member)                     | = | 03 (in progress) |
| <i>M.Phil. Students (As a Main Supervisor)</i>             | = | 200 (completed)  |
| M.Phil. Students (As a Main Supervisor)                    | = | 19 (in progress) |
| BS/M.Sc. Technical report Students (As a Main Supervisor)  | = | 51 (Completed)   |
| <i>BS Technical report Students (As a Main Supervisor)</i> | = | 60 (Completed)   |
| BS Technical report Students (As a Main Supervisor)        | = | 10 (in progress) |

## RESEARCH PAPERS/ BOOKS PUBLISHED

|                                              |    |
|----------------------------------------------|----|
| Abstracts                                    | 15 |
| Conferences/Workshops /Trainings             | 60 |
| PATENTS                                      |    |
| Patents submitted (submitted & under review) | 02 |

- a. Entitled as **“Development of the Calibration procedure for Stopwatch/Timer Calibration in line with ISO: IEC 17025”**, Dr. Abdul Qayyum Khan†, Dr. Ghalib-Ul-Islam\*, Dr. Shafiq-Ur-Rehman, Dr. Shamsa BiBi, Dr. Zeeshan Ali submitted on **16<sup>th</sup> august 2025** by Applied Physics Computers and Instrumentation Center (APC&IC) Pakistan Council of Scientific and Industrial Research (PCSIR), Laboratories Complex Lahore 54600 Pakistan.
- b. Entitled as **“A process for pH meter calibration with milivolts source”**, Dr. Abdul Qayyum Khan, Dr. Muhammad Zia-ur-Rehman, Dr. Shafiq-Ur-Rehman, Dr. Shamsa BiBi, Dr. Rashid Jalil, Dr. Muhammad Imran Jamil, Dr. Ghalib-Ul-Islam, Sajjad Ahmad. Submitted by Applied Physics Computers and Instrumentation Center (APC&IC) Pakistan Council of Scientific and Industrial Research (PCSIR), Laboratories Complex Lahore 54600 Pakistan.

## Book Chapters

- o Haq Nawaz Bhatti and Saima Noreen, **2017**. Principles of Environmental Chemistry. The Caravan Book House Lahore (**Chapter # 02-** Atmospheric Chemistry).

- Haq Nawaz Bhatti and Muhammad Salman, 2017. Applied Chemistry. The Caravan Book House Lahore (**Chapter # 11 & 12** Dyes, Paints and Pigments-Paper and Leather Industries).

#### **ADDITIONAL ADMINISTRATIVE SERVICES (03)**

- i. Acted As **“Deputy Hall Warden (Female) “PARS, UAF from 01/09/2023 to March 2026).**
- ii. Acting as **Superintendent of Arnic Hall, PARS** from 26/10/2022 to date.
- iii. Acting as Superintendent of **Khalid Hall, PARS** from 24/06/2025 to date.
- iv. Acting as **Hall Superintendent to CHE female, PARS from 21/09/2025** to 07/01/2026.
- v. Acted As **“Deputy Hall Warden (Female) “PARS, UAF from 08/01/2026 to date).**
- vi. **Co-Tutor** of Qasim-3, at UAF Community College, PARS from 26/10/2022 to date.
- vii. Acting as **Departmental Website Focal Person** for department of Chemistry from June 2023 to date.
- viii. Acting as **Departmental QEC Focal Person for department of Chemistry** from June 2025 to date.

#### **ADMINISTRATIVE SERVICES ASSIGNED BY DEAN/ DIRECTOR/ CHAIRMAN ON ANNUAL BASIS**

- i. Acting as **member of BOS Department of Chemistry**, University of Agriculture Faisalabad, Pakistan since October 2015.
- ii. Acting as **member of Academic Council, University of Agriculture Faisalabad**, Pakistan since June 2024.
- iii. Acted as **Female Advisor for undergraduate students** at department of Chemistry from 01/09/2022 to June 2025).
- iv. Acting as **Departmental Website Focal Person** for department of Chemistry from June 2023 to date.
- v. Acting as **Departmental QEC Focal Person for department of Chemistry** from June 2025 to date.
- vi. Acting as **Departmental OBE Focal Person** for department of Chemistry from October 2025 to date.
- vii. Acting as **Departmental PEER-QEC Conveyer** of committee from 12/11/205 to date.
- viii. Acting as **CO-Organizer of Chemical Society, at department of Chemistry** September 2022 to date.
- ix. Acting as member of **“Course Review and Course File Committee”** of Chemistry Department from 01/07/2022 to date).
- x. Acted as **Manager for Squash Female Team, Faculty of Sciences, UAF Sports League 2021-2022.**
- xi. Acted as **Coach for Cricket Female Team, Faculty of Sciences, UAF Sports League 2023-24.**
- xii. Acted as Committee member of team for **“Chinese Delegation Visit at UAF about QINCHAIINSTITIUTE OF SALT LAKES INEST ABLISHING A RESEARCH CENTER OF HIMALAYAN ROCK SALT IN PAKISTAN”.**
- xiii. Acted as, **In charge of the ‘Female Students Matters Committee’** at UAF Community College PARS 2016-2018.

#### **COMMUNITY SERVICES**

- a) ***Duty performed in wheat campaign*** by University of Agriculture Faisalabad by collaboration with **‘Punjab Government Agriculture department extension’** from 08 -15th November 2025.
- b) ***Performed Election Duty As “Presiding Officer”*** during General Elections of Pakistan, 8th February 2024.
- c) ***Duty performed in wheat campaign*** by University of Agriculture Faisalabad by collaboration with **‘Punjab Government Agriculture department extension’** from 12 -20th November 2021.

- d) *Performed Election Duty As “Presiding Officer”* during General Elections of Pakistan, 2018.

### **ACTING AS REVIEWER**

#### **As journal Editor/referee**

1. **Acting as “Journal CO-Guest Editor”** for journal “*Frontiers in Chemistry*” research topic entitled as “*Molecular System Theoretical Calculations for Organic Electronics*” year 2023 to date.
2. Acting As a Reviewer for “Advances in Science, Technology and Engineering Systems Journal (ASTESJ)” from Oct 2017.
3. Acting as Referee for “IOP Science” from April 5<sup>th</sup>, 2019.
4. **Acting as a Reviewer** for “World Journal of Surgical Oncology” from June 2019 to date.
5. **Acting as a Reviewer** for “*Fibers and Polymers*” from 2021 to date.
6. Acting as a Reviewer for “*Polymer for Advanced technologies by Wiley*” from 2021 to date.
7. Reviewer for Journal “*Results in Chemistry*” (from 28 July 2022-Present).
8. **Acting as a Reviewer for “Computers in Biology and Medicine” by from March 2024 to date.**

#### **Acted as an External Reviewer for the review of the PREE/SAR Year Report**

- I. Acted as an External Reviewer for the review of the PREE/SAR Year Report for the BS Chemistry program at the Department of Chemistry, Government College Women University Faisalabad (GCWUF), held on 28th May 2026.
- II. Acted as external Reviewer for “Review Report of PREE/SAR year” GCWUF for the programs of M.Phil. Chemistry on 28th May 2026.
- III. Acted as external Reviewer for “Review Report of PREE/SAR year” GCWUF for the programs of Ph.D. Chemistry on 28th May 2026.
- IV. Acted as external Reviewer for “Review Report of PREE/SAR year” GCWUF for the programs of BS Forensic Science on 28th May 2026.

#### **M. Phil Thesis evaluation (Acting as External Examiner)**

##### **2026**

- i. As External Examiner of student names” Nimra Zahoor” 2024-GCUF-01295, Session 2024-2026 of M.Phil. entitled as “Computational Studies of Leas Free Halide Double Perovskite Materials” at Department of Chemistry, GC University Faisalabad (30 June 2026).
- ii. As External Examiner of student names” Arshia Irfan” Roll No. CIIT/SP24-R06-003/LHR, Session 2024-2026 of M.Phil. entitled as “Transition Metal Doped B12 N12 Nanocage as Single Atom Catalyst for Nitrogen Reduction to Ammonia: A DFT Study” at Department of Chemistry, COMSATS University Islamabad, Lahore Campus-Pakistan. (6 Jan 2026).
- iii. As External Examiner of student names” Muqaddis Zahra” Roll No. CIIT/SP24-R06-012/LHR, Session 2024-2026 of M.Phil. entitled as “Exploring Metal Doped B12 N12 Nanocage as single Atom Catalyst for CO2 Reduction to Formic Acid: A DFT Driven Analysis” at Department of Chemistry, COMSATS University Islamabad, Lahore Campus-Pakistan. (6 Jan 2026).
- iv. As External Examiner of student names” Syed Muhammad Zareef” Roll No. CIIT/SP24-R06-023/LHR, Session 2024-2026 of M.Phil. entitled as “Enhanced Hydrogen Storage and Dissociation on Metal Doped g-C3N4 via

Electric Field Modulation: A DFT Study ” at Department of Chemistry, COMSATS University Islamabad, Pakistan. (6 Jan 2026).

#### **2025**

- v. As External Examiner of student names” Fatima Islam” Roll No. 230875, Session 2023-2025 of M.Phil. entitled as “synthesis and Anti-inflammatory activity of derivatives of 2-(3-benzophenyl) propanoic acid” at Department of Chemistry, GC University, Faisalabad. (August 2025).
- vi. As External Examiner of student names” M. Kamran Irshad” Roll No. 230887, Session 2023-2025 of M.Phil. entitled as” Mineral Profile and Biological Evaluation of Dianella Tasmanica Variegata Leaves” at Department of Chemistry, GC University, Faisalabad. (August 2025).
- vii. As External Examiner of student names” Maria Hussain” Roll No. 230869, Session 2023-2025 of M.Phil. entitled as” synthesis and Anti-inflammatory activity of thiophene based oxadiazole derivatives” at Department of Chemistry, GC University, Faisalabad. (August 2025).
- viii. As External Examiner of student names” Hareem Jabbar” Roll No. 231689, Session 2023-2025 of M.Phil. entitled as”” at Department of Chemistry, GC University, Faisalabad. (November 2025).
- ix. As External Examiner of student names” Aqsa Bano” registration no. 2023-GCWUF-0103, Session 2023-2025 of M.Phil. entitled as “Spectroscopic analysis of substituted cyanuric Chloride by using computational studies.” at Department of Chemistry, GCW University, and Faisalabad (viva held on October 2025).

#### **2024**

- i. As External Examiner of student names” Amina Parveen” ID no. MSF2204539, Session 2022-2024 of M.Phil. entitled as” Surface -enhanced Raman spectroscopy for characterization of residue and filtrate portions of blood serum samples of breast cancer.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (June 2024).
- ii. As External Examiner of student names” Rahila” ID no. MSF2204537, Session 2022-2024 of M.Phil. entitled as” NMR Cyclic Volumetry and Dynamic Light Scattering Study (DLS) Of Microemulsion System.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (July 2024).
- iii. As External Examiner of student names” Muhammad Ahsan Jawad” Roll no. 2221201, Session 2022-2024 of M.Phil. entitled as” Synthesis characterization and biological evaluation of Naphthalene-1-amine based ligands and their metal complexes.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (October 2024).

#### **2022**

- iv. As External Examiner of student names” Fazeelat” registration no. 2016-GCWUF-2665, Session 2020-2022 of M.Phil. entitled as” Development of oleo gels: promotion of healthy skincare products” from wastepaper: experimental and theoretical studies.” at Department of Chemistry, GCW University, and Faisalabad (viva held on 22nd November 2022).
- v. As External Examiner of student names” Kinza” registration no. 2017-GCWUF-0945, Session 2019-2021 of M.Phil. entitled as” Strengthening adsorption process for water contaminated by pharmaceutical compounds using cellulose derived from waste paper: experimental and theoretical studies.” at Department of Chemistry, GCW University, and Faisalabad (January 2022).

#### **2021**

- vi. As External Examiner of student names” Rabia Tabassum” Roll No. 509, Session 2019-2021 of M.Phil. entitled as” Synthesis and Characterization of Lead-Free Halides Double Perovskite Materials” at Department of Chemistry, GC University, Faisalabad. (November 2021).
- vii. As External Examiner of student names” Tayyba Shoukat” Roll No. 601, Session 2019-2021 of M.Phil. entitled as” Facile Synthetic Routes of Graphene Quantum Dots from Indigenous Coal And Their Characterization” at Department of Chemistry, GC University, Faisalabad. (December 2021).
- viii. As External Examiner of student names” Saba Yaqoob” Roll No. 613, Session 2019-2021 of M.Phil. entitled as” Synthesis, Antibacterial and Insilico Modeling of Novel Oxadiazole Derivatives As Potential Therapeutics” at Department of Chemistry, GC University, Faisalabad. (December 2021).

## **2020**

- ix. As External Examiner of student names” Sundus Aziz” Roll No. 1013-GCWUF-0779, Session 2018-2020 of M.Phil. at Department of Chemistry, GCW University, Faisalabad.
- x. As External Examiner of student names” Ajmal Shezad” Roll No. 395333, Session 2018-2020 of M.Phil. at Department of Chemistry, GC University, Faisalabad.
- xi. As External Examiner of student names” Farwa Khalid” Roll No. 1014-GCWUF-1931, Session 2018-2020 of M.Phil. at Department of Chemistry, GCW University, Faisalabad.
- xii. As External Examiner of student names” Zainib Razzaq” Roll No. 614, Session 2019-2021 of M.Phil. at Department of Chemistry, GC University, Faisalabad.

## **2019**

- xiii. As External Examiner of student names” Mr. Rizwan Ali Roll No. 26401, Session 2017-2019 of M.Phil. at Department of Chemistry, GC University, Faisalabad.

## **PhD Comprehensive Examiner**

## **2026**

- i. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Unha Tahir, Reg No. 2016-ag-3101” held on 10/11/2022 at 2: 30 pm, in the Video Conference Room (DFS) UAF.
- ii.
- iii. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Unha Tahir, Reg No. 2016-ag-3101” held on 10/11/2022 at 2: 30 pm, in the Video Conference Room (DFS) UAF.
- iv. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Arifa Murtaza, Reg No. 2015-ag-1035” held on 24/11/2022 at 2: 30 pm, in the Video Conference Room (DFS) UAF.
- v. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Arooj Fatima, Reg No. 2018-ag-4031” held on 06/11/2022 at 11 am, in the Video Conference Room (DFS) UAF.
- vi. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Mr. Ghulam Mustafa, Reg No. 2015-ag-3586” held on 16/07/2021 at 2pm, in the Video Conference Room DLC-I UAF.

### **Details PhD Thesis completed = 03**

#### **As Major Supervisor**

Tazeem Fatima (2014-ag-9811), "Quantum chemical study of organic chromophores for design linear and non-linear optical materials", February 2026

Sania Ismaeel (2017-ag-0566) "Theoretical investigation of high performing donor materials for organic photovoltaics", April 2026.

- Hafsa Majeed (20219-ag-2220), "Computational Study to Design Potential Carriers in drug delivery system" (thesis submitted).

#### **As member**

- Huma Shamshad (2018-ag-4007), "Fabrication and Characterization of green Nano biopesticides as an ecofriendly approach for pest control".
- Rida Fatima (2018-ag-3922), "Designing of efficient hole transport materials for applications in third generation solar cells".

### **1. PhD Thesis Ongoing (Comprehensive Examination is Done)**

#### **As major Supervisor = 03**

- Sofia Faiz (2019-ag-2246), "Computational Insights into Anticancer Drug Designing for Breast Cancer Treatment".
- Sidra Moeed (20021 ag-1683), "DFT Based Strategies for Designing High Performance Small Molecular Solar Cell Materials".

#### **As Member = 01**

### **2. Ph.D. Theses (synopsis defended one time)**

#### **As major Supervisor = 01**

- Sadiya Sadiq

As member= 05

- Hamza physics (2020-ag-1432), "Layard double Hydroxide materials for energy Storage devices".
- Nimra Asif (2022-ag-2183), "Multiferroic optical and thermoelectric properties of dopped perovskite materials by density functional theory".
- Muhammad Ramdan (2017-ag-4709), "Theoretical investigation of Cosmic Rays propagation in Plasma: applications in Astro physical Environment".
- Mahnoor
- Maheen

### **Details of Technical report students-completed year wise**

#### **M.Sc. Chemistry Technical Reports**

##### **Session: 2015-2017**

1. Samra Nadeem (2015-ag-2290) "*Performance of acceptor material of organic solar cell*"
2. Sawaira Shahid (2015-ag-1720) "*Applications of OLD's*"
3. Anum Javed (2015-ag-2439) "*Energy crisis*"
4. Arslan Bashir (2015-ag-3666) "*Organic light emitting diode and applications*"

5. Fatima Baig (2015-ag-3351) *"Performance of organic and inorganic solar cell material"*
6. Ayesha Akram (2015-ag-2493) *"Structure, types, materials of OLD's"*
7. Fatima Shahid (2015-ag-1386) *"Structure, properties and fabrication of inorganic solar cell"*
8. Hussain Ferid Sabri (2015-ag-2656) *"Renewable and non-renewable energy sources"*
9. Khalid Ahmed (2015-ag-2626) *"Solar energy and its applications"*
10. Nadia Ashfaq (2015-ag-3700) *"Structure, properties and fabrication of organic solar cells"*
11. Shahida Ashraf (2015-ag-3076) *"Development in the field of solar cells"*
12. Zill-e-Huma (2015-ag-3035) *"Computational chemistry"*

#### Session: 2016-2018

1. Muhammad Noman (2016-ag-1112) *"Solar cells industry"*
2. Hanna Zulfiqar (2016-ag-3535) *"Chemistry of Cosmetics"*
3. Noor ul Lain (2016-ag-3537) *"Effective waste management approach"*
4. Iqra Shakoor (2016-ag-1675) *"Acceptor materials for organic solar cell"*
5. Kawasah Javed (2016-ag-1776) *"PDI derivatives as acceptors for organic solar cell"*
6. Safoora Saleem (2016-ag-3178) *"Chemical sensors"*
7. Abdul Salam Mudassar (2016-ag-2410) *"Bioenergy"*
8. Tayyaba Rafiq (2016-ag-996) *"Biodiesel"*
9. Farwa Aslam (2016-ag-1763) *"Nanomedicine"*
10. Muhammad Farman (2016-ag-2701) *"Chemistry and biochemistry of sleeping"*
11. Samreen Naz (2016-ag-1434) *"Chemical reagents and their chemistry"*
12. Sadia Zulfiqar (2016-ag-473) *"Energy crises in Pakistan"*
13. Ayesha Akram (2016-ag-2493) *"Organic light emitting diodes"*

#### Session: 2017-2019

1. Muhammad Salman Usaid (2017-ag-4506) *"Green Chemistry"*
2. Samra Shakeel (2017-ag-4768) *"Honey Used as Medicine in Ancient and Modern era"*
3. Kainat Fatima (2017-ag-5276) *"Biochemistry of Skin and its Diseases"*
4. Mehreen Safdar (2017-ag-4483) *"Electropolishing"*
5. Shamsa Kanwal (2017-ag-5501) *"Chemistry of Bentonite Clay and its applications in our Life"*
6. Awais Ahmad (2017-ag-4487) *"Gliding"*
7. Muhammad Usman (2017-ag-5291) *"Chemical Sensors in Human Body"*
8. Abdul Khaliq (2017-ag-4507) *"Solar Cell Industry in Pakistan"*
9. Misbah Abid (2017-ag-5278) *"Quality of Water in Pakistan"*
10. Safeer Mahdi (2017-ag-5468) *"Computational Chemistry"*

#### Session: 2018-20

1. Muhammad Farhan Farid (2018-ag-793) *"The Comparison between green and chemical synthesis"*
2. Aneel Allyas (2018-ag-889) *"Chemistry of Explosive Materials and their Mechanisms"*
3. Hafsa Naz (2018-ag-632) *"Brief discussion of antibiotics"*
4. Farhat Shah Nawar (2018-ag-5575) *"Use of chocolate as a medicine"*
5. Khuram Shahzad Maqbool (2018-ag-839) *"Bio-Diesel and its uses"*
6. Sayed Irfan Haider Shah (2018-ag-765) *"Chemistry of black and white and colored photography"*
7. Aqsa Hameed (2018-ag-635) *"Chemistry of Metabolism in Human beings"*

8. Sadia Naz (2018-ag-4775) *"Chemistry of blood groups"*
9. Sidra Latif (2018-ag-4574) *"Carcinogenic Effects of Junk Food"*
10. Tehzeeb Zara (2018-ag-815) *"Cancer causes and cure"*
11. Asma Akhtar (2018-ag-636) *"Role of antioxidants in our body"*
12. Iqra Afzaal (2018-ag-794) *"Water Pollution and their Removal methods"*
13. Usama Riaz (2018-ag-623) *"Role of Antibiotics"*
14. Usama Qadeer (2018-ag-718) *"Brief discussion of periodic table of elements"*
15. Amna Shabir (2018-ag-841) *"Metal based anti-cancer drugs"*
16. Sabahat Javed (2018-ag-876) *"Diabetes is a silent killer"*.

### **BS CHEMISTRY Technical Reports**

#### **Session 2019-2023**

1. Rida Tufail (2019-ag-5553) *"Green Aspiration Level ' A New Green Chemistry Metric"*
2. Aima (2019-ag-5715) *"Nanotechnology in Cosmetics"*
3. Muhammad Burhan (2019-ag-5578) *"Depression"*
4. Muhammad Amin (2019-ag-5676) *"Importance of Inorganic Chemistry in Daily Life"*
5. Iqra Shaheen (2019-ag-5603) *"Pharmaceutical Powder Handling"*
6. M. Aamash (2019-ag-5588) *"Dynamite and Explosive Materials"*
7. Zain-ul-Abideen (2019-ag-5519) *"Carbon Footprints"*
8. Ayesha Ashfaq (2019-ag-5705) *"Chemistry of Schiff Bases"*
9. Amna Zafar (2019-ag-5711) *"Solar Cells and Industry"*
10. Sadia Siddique (2019-ag-5546) *"Dates and Palm Varieties and their Nutritional Value"*
11. Umar Hassan Basheer (2019-ag-5649) *"Fuel Cell Efficiency and Potential for Improving Energy Sustainability"*
12. Zainab Abid (2019-ag-5645) *"Role of Chemistry in Cancer Research and Treatment"*
13. Eimad-U-Deen (2019-ag-5618) *"Green Chemistry in Food and agriculture Science"*
14. Asmat Ullah (2019-ag-5624) *"Role of Graphene Based Nano Carriers in Drug Delivery"*
15. Taiba Liaqat (2019-ag-5655) *"Pathogenesis and Etiology of Renal Calculi; An Overview of the Different Types of Stones and the Factors that Contribute to their formation"*

#### **Session 2020-2024**

#### **BS Chemistry (2020-2024)**

1. Amna Aslam (2020-ag-9358) *"Pulp and paper chemistry"*
2. Atsha Maryam Wajid (2020-ag-9364) *"Chemistry of emotions"*
3. Emaan Tahir (2020-Aag-9370) *"Food packaging"*
4. Hadia Sadiq (2020-ag-9376) *"Forensic science and chemistry"*
5. Kashaf Yaqub (2020-ag-9396) *"Enzymes in human body"*
6. Mudasir Hussain (2020-ag-9415) *"New trends in nuclear chemistry with manufacturing of nuclear material"*
7. Aftab Akhtar (2020-ag-9462) *"Chemistry in spices"*
8. Amina Amjad (2020-ag-9477) *"Polymers and its applications in daily life"*
9. Anam Mustafa (2020-ag-9483) *"Role of metal and non metal in our body"*
10. Farhat Hussain (2020-ag-9511) *"Chemistry in dairy products"*

11. Farrah Riaz (2020-ag-9513) "Forensic science and Chemistry"
12. Iqra Fatima (2020-ag- 9527) "Chemistry of baking"
13. Malaika Shoukat (2020-ag-9540) "Chemical and biopesticides"
14. Muhammad Shaban Munir (2020-ag-9571) "Solar Industry"
15. Muhammad Toqeer Jabbar (2020-ag-9575) "Chromatography and its Advanced Types"
16. Nooreman (2020-ag-9589) "Smog and cloud seeding"
17. Shahzaman (2020-ag-9602) "Rubrics for Science lab/Laboratory report"

#### **Technical Report Students 2021-2025**

18. Zoha Khan (2021-ag-8792), Chemical Aspects of Nutraceutical.
19. Amna Khalil (2020-ag-9172), From Kitchen to Medicine: The Invisible Hand of Chemistry in Daily Life.
20. Hira Anum (2021-ag-8729), Fragrance Chemistry
21. Rubab Shahid (2021-ag-8767), Plastic Pollution
22. Amna Nasim (2021-ag-8610), Analysis of Pesticides Residues in Fruits and Vegetables.
23. Roshna Zaka (2021-ag-8674), Food Ingredients Impact on Skin Health
24. Zarmeen Ahmad (2021-ag-8697), AI and Chemistry
25. Zuha Khalid (2021-ag-8701), Chemistry of Aging
26. Laiba Aziz (2021-ag-8638), Microplastic as An Adsorbent to Remove Pollutants from Aqueous Bodies.
27. Muhammad Farooq Khan (2021-ag-8655), Greenhouse Gases, Impact Source and Solutions.
28. Raza (2021-ag-8659), Physical Testing of Paper and Board.

#### **Technical Report Students 2022-2026**

29. Mehak Ashraf (2022-ag-5138) "Chemical Composition and Health Risks of E-Cigarettes and Vaping Liquids"
30. M. Talha Jameel (2022-ag-5148) "Chemical Composition of Different Shampoos and Soaps"
31. Saba Tariq (2022-ag-5159) "Ultrasensitive Electrochemical Sensing of PFAS in Water"
32. Amna Amin (2022-ag-5186) "Nutritional Supplements vs. Natural Food Sources: A Chemical and Bioavailability Perspective"
33. Dua Fatima (2022-ag-5230) "Antimicrobial Resistance and the Overuse of Antibacterial Household Products"

#### **Details of MPhil Students-completed year wise**

##### **MPhil Chemistry Research**

##### **Session: 2015-17**

1. Ahmed Waqas (2015-ag-2607) "Effect of Substitutions on the Optical and Charge Transfer Properties of Small Molecular Donors for Organic Light Emitting Diodes"
2. Anam Yasin (2015-ag-3433) "Study of Optical Properties of Different Small Molecular Donor Materials for Organic Solar Cells"
3. Asma Alam (2015-ag-2998) "Effect of Substitution on Optical and Charge Transfer Properties of Diketopyrrole-Based Small Molecules as Donating Materials for Organic Solar Cells (OSCs)"
4. Sufian Afzal (2015-ag-3309) "Study the Effect of Substitutions on the Optical and Charge Transport Properties of Small Donor Materials for Organic Light Emitting Diodes"
5. Sundas Shafiq (2013-ag-716) "Study of Optoelectronic Properties of Thiophene Based Organic Donor Material for Solar Cells"
6. Tahira Jeelani (2015-ag-3175) "Designation and Investigation Small Donor Molecules for Organic Solar Cell"

##### **Session: 2016-18**

1. Farhat Noor (2016-ag-1626) "DFT studies on optoelectronic characterization of acridine and carbazole derivatives for organic dye-sensitized solar cell"
2. Arif Shafiq (2016-ag-3197) "Theoretical investigation of donor bipolar molecules with 1,8 naphthalimide and triphenylamine moieties as organic light emitting materials"
3. Sana Bakhtawar (2014-ag-8725) "Biodiesel production from castor oil using different catalysts: process optimization"
4. Khadija Tahir (2014-ag-9279) "A computational study of narrow band gap benzodipyrrolidone based donor conjugated polymers"
5. Arifa Kousar (2016-ag-1467) "Computational study of benzo[1,2-b:4,5-b'] dithiophene based fluorescent materials for organic light emitting diodes (OLEDs)"
6. Munazza Naseem (2016-ag-775) "Evaluation of castor seed biomass for bioenergy production and waste water treatment"
7. Shah Bano (2014-ag-2603) "Density functional studies of charge transfer properties of bithiophene based electron donors in organic solar cells"
8. Faiza (2016-ag-1795) "Diketopyrrolopyrrole based small molecules as donating material for organic solar cells"
9. Nazia (2016-ag-2124) "Preferential cyclotrimerization of 5-(Aminomethyl)-2- furan carboxylic acid: electrostatic and orbital interaction studies"
10. Muhammad Shoaib (2016-ag-304) "Designation of acceptors to match with donors molecules via substitutions of perylene diimide for organic solar cells"
11. Ushna Saeed (2016-ag-112) "Effect of electron donating and electron withdrawing groups on optoelectronic properties of perylene diimide (PDI) based small molecules for organic solar cells"

#### Session: 2017-19

1. Memoona Saleem (2017-ag-3272) "Theoretical Investigation to Study Photovoltaic Properties of Non-Fused Small Molecule Acceptor"
2. Muhammad Ahsan Jameel (2017-ag-3278) "Treatment of Black Liquor by Graphene Oxide"
3. Musfira Riaz (2014-ag-3185) "Theoretical Investigation of Carbazole Based Dyes for Organic Photovoltaics"
4. Dur-e-Nayab (2017-ag-3194) "Process Optimization of Biodiesel Production from Safflower Seed Oil"
5. Fiza Hussain (2017-ag-5152) "A Computational Investigation of Organic Dye-sensitized Solar Cells"
6. Muhammad Slaman Sahota (2017-ag-3190) "Effect of Various Substituents on the Large Energy Gap Between Triplet Excited-States of Naphthalene"
7. Saman Naz (2017-ag-3192) "Computational Study to Know the Effect of Aromatic Rings on Solar Cells Materials"
8. Shaista Ghafoor (2017-ag-3122) "Non-Fullerene Metal Donor-Acceptor Material for Organic Solar cells"
9. Sobia Iqbal (2017-ag-3294) "Treatment of Black Liquor by Charcoal"
10. Syed Ali Haider Naqvi (2017-ag-3149) "Theoretical Investigation of Photovoltaic Properties for Star Shaped Organic Donor Solar Cells Materials"
11. Shaista Ghafoor (2017-ag-3122) "Non-Fullerene Metal Donor-Acceptor Materials for Organic Solar Cells"
12. Saman Naz (2017-ag-3192) "Computational Study to know the effect of aromatic rings on solar cells materials"
13. Muhammad Ahsan Jameel (2017-ag-3278) "Treatment of Black Liquor by Graphene oxide"
14. Musfira Riaz (2014-ag-2185) "Theoretical investigation of Carbazole based dyes for Organic Photovoltaics"
15. Fizza Hussain (2017-ag-5152) "Computational Investigation of organic dyes sensitize solar cells"
16. Muhammad Salman Sahoota (2017-ag-3190) "Effect of various substituents on the large energy gap between triple excited states of naphthalene"
17. Dur-e-Nayab (2017-ag-3194) "Process optimization of biodiesel production from safflower seeds oil"
18. Syed Ali Haider Naqvi (2017-ag-3149) "Theoretical Investigation of Photovoltaic properties for Star shaped organic Donor Solar cells materials"
19. Sobia Iqbal (2017-ag-3294) "Treatment of Black liquor by Charcoal"

#### Session: 2018-2020

1. Rimsha Irshad (2018-ag-3904) "Designation of efficient 3-Hydroxychromone based donors organic photovoltaics"
2. Fabiha Bushra (2018-ag-4035) "Designation of donor materials via substitutions of different donor-acceptor groups for organic photovoltaics"
3. Amer Naseem (2018-ag-3991) "Computational study of high performance materials for organic light-emitting diodes"
4. Muhammad Uzair Riaz (2016-ag-1835) "Computational study of thermally activated delayed fluorescence materials for organic light-emitting diodes"
5. Shazia Javed (2018-ag-4579) "Theoretical study of high performing organic solar cells materials"
6. Bushra Kanwal (2018-ag-4713) "Theoretical study of organic dyes to investigate the effects of a  $\pi$  spacer on donor-acceptor molecules"
7. Ammara Naseem (2018-ag-3878) "Computational study of TiO<sub>2</sub>-flavylium based dye-sensitized solar cells"
8. Faiza Farooq (2018-ag-3805) "Theoretical study of optical and electrochemical properties of phenothiazine based derivatives as fluorescent materials"
9. Sidra Ijaz (2018-ag-3897) "Computational study of D- $\pi$ -A organic dyes for dye-sensitized solar cells based on 8, 9, 10-trimethoxydibenzo [b, h] [1, 6] naphthyridine"
10. Siddra Shafiq (2018-ag-3975) "Computational study of substitutional effects of diphenyl pyrimidine for OLEDs"
11. Misbah Aslam (2018-ag-4029) "Computational investigation of antioxidant capacity of petunidin based drugs"
12. Tanzila Mumtaz (2015-ag-2477) "Molecular design of donor-acceptor dyes for dye-sensitized solar cells a DFT study"
13. Javeria Ashraf (2018-ag-4002) "Theoretical investigation of TADF materials via CN/H substitutions in phenothiazine based molecules"
14. Sundas Saleem (2018-ag-4008) "Computational investigation of fluorescein based dyes for dye-sensitized solar cells"
15. Amna Saleem (2018-ag-4023) "Designation of higher performance 3-hydroxychromone based donor molecules for organic solar cells"
16. Muhammad Usman Tahir (2018-ag-3879) "Acetic Acid pulping of Bamboo strips"
17. Nafeesa Shahbaz (2018-ag-3822) "Series of Organic Light Emitting Diodes emitter for thermally activated delayed fluorescence"
18. Urwa Tahir (2018-ag-4022) "Computational study of optoelectronic properties of High Performance Materials for OLEDs"
19. Palwasha Tehseen (2018-ag-3885) "Theoretical investigation of anthocyanin based dyes for organic photovoltaics"
20. Hafiz Mohsin Shazad (2018-ag-3881) "Alkaline pulping of Bamboo Chips with Sodium Carbonate"

#### Session: 2019-21

1. Laryeb Khalid (2019-ag-2285) "DFT investigations of the adsorption of gemcitabine anticancer drug on transition metal doped boron nitride fullerenes"
2. Shumaila Sadaf (2019-ag-2200) "Computational study of selenium substituted donor- acceptor-donor based polymer for solar cells"
3. Faiza Shafiq (2019-ag-2279) "Computational analysis of pyrazine based TADF materials"
4. Sana Sajjad (2019-ag-3571) "Designation of Azo based derivatives for organic solar cells as acceptor materials"
5. Hafsa Majeed (2019-ag-2220) "Theoretical study of 8-Quinolinolato-Alkali based, Electron Transporting Materials for OLED Devices"
6. Hafiza Aqsa Ali (2019-ag-2254) "DFT study of various anticancer drugs for pharmaceutical applications"
7. Shahzad Ahmed Saeed (2017-ag-551) "Effect of different pi-spacers in Triphenylamine based Dyes for Dye-sensitized solar cells: A Computational Study"
8. Fatima Sarwar (2017-ag-618) "Computational designing of push-pull chromophores to tune their nonlinear optical properties"
9. Maimoona Zia (2019-ag-2276) "Exploring the potential of novel phenolic compounds as potential therapeutic drug against SARS-CoV-2 through DFT and molecular docking"
10. Muhammad Rizwan Asghar (2019-ag-2262) "Cyclopentadithiophene CPDT based small molecules for highly efficient blue emitters in OLEDs :A DFT study"

11. Sehrish Iftikhar (2015-ag-184) "Characterization and theoretical study of naphthodithiophene based donor materials for Organic solar cells"
12. Amna bibi (2019-ag-2210) "Quantum chemical study of the heterocyclic compounds for efficient optical and nonlinear optical properties"

#### Session: 2020-22

1. Aamna Saleem (2020-ag-1158) "Fragmentation mechanisms of secnidazole by advanced oxidation processes; DFT Study"
2. Mohammad Bilal (2020-ag-1159) "Computational study of cyclopentadithiophene based derivatives for organic light-emitting diodes"
3. Hammad Aslam (2018-ag-700) "A DFT study of diketo-pyrrolopyrrole based small molecules for organic solar cell application"
4. Gulzaib Basharat (2020-ag-1227) "The impact of solvent on the photochemical properties of anticancer drug PLX4720, A computational study"
5. Anum Saeed (2020-ag-1249) "Hexagonal boron nitride nanosheet as drug delivery system for anticancer drugs"
6. Nimra Zahir (2020-ag-1218) "Identification of ketone derivatives as potent inhibitors of estrogen receptor alpha of breast cancer. An in-silico study"
7. Faiqa Liaqat (2016-ag-2245) "Substitution effect of donor fragment on optoelectronic properties of organic photovoltaic materials"
8. Mahnoor Tariq (2020-ag-1177) "Theoretical study of interaction of various antihypertensive drugs with DNA base pairs"
9. Ramish Ramzan (2020-ag-1184) "Designing of donor-acceptor low bandgap monomers for polymer solar cells by DFT study"
10. Sara Muslim (2018-ag-658) "Computational studies on optoelectronic and charge transfer properties of material for dye sensitized solar cell applications"
11. Yasmeen Iqbal (2020-ag-1243) "Small molecule acceptors for organic solar cells applications"
12. Mafia Ashraf (2020-ag-1236) "Computational study of small molecules for organic light-emitting diode"

#### Session: 2021-2023

1. Aqsa Atique (2021-ag-1602) "Comparison of Carbon-X Based Nanocones for Flutamide Adsorption: A DFT Study"
2. Tehmeena Batool (2021-ag-1677) "Zinc Carbide Based 2D Monolayers as Drug Delivery System: A Computational Study"
3. Nadia Munawar (2021-ag-1614) "Removal of Dyes from Wastewater Using Silica Gel-Graphene Oxide Composite: A DFT Study"
4. Mubarra Anwar (2021-ag-1722) "Computational Studies of a Schiff base Based on Sulfonamide"
5. Amna Nasir (2021-ag-1715) "Structural, Spectral, Computational Study of 5BRSDA from 5-Bromosalicylaldehyde and Sulfadiazine"
6. Laraib Shahid (2021-ag-1714) "Cellulose and Sodium Alginate Composite for the Removal of Malachite Green Dye: DFT Studies"
7. Fizza Shahzad (2021-ag-1645) "A DFT Study of Nanocones as a Drug Delivery Carrier with Flutamide Drug"
8. Fatima Kausar (2021-ag-2667) "Zinc Carbide Nanosheet as Drug Delivery System; DFT Study"
9. Aneeqa Sattar (2021-ag-3063) "Computational Study of Thermally Activated Delayed Fluorescence Materials"
10. Muhammad Abdullah (2019-ag-3302) "DFT Study of Organic Light-Emitting Diodes"
11. Saba Ashraf (2021-ag-2583) "Configuration Analysis of Furan II-Spacer and their Hypocritical Effect on INDOL [3, 2, 1-JK] Carbazole-Based Dye-Sensitized Solar cells Materials"
12. Alishba Khalid (2021-ag-2591) "Non-Linear Optical (NLO) Materials: A DFT Study"
13. Jannat Mehboob (2021-ag-2612) "A Computational Study of Small Donor Molecules for Solar Cells"
14. Zeshan Sarwar (2021-ag-2702) "Theoretical Study of Organic Light Emitting Diodes"
15. Zeeshan Bashir (2021-ag-2704) "DFT Analysis of Small Molecules for Organic Solar Cells"

16. Rabia Amin (2018-ag-737) "Molecular Docking and DFT Study of Antiproliferative Agents"
17. Rabia Qayyum (2018-ag-777) "Designing of Small acceptor Molecules for Organic Solar Cells"
18. Rabiya Irshad (2021-ag-2626) "DFT Studies of Nanocages for Targeted Delivery of Drugs"
19. Aneeqa Kanwal (2021-ag-2627) "DFT Study of Materials for Organic Photovoltaic Devices"
20. Muhammad Hasnain (2021-ag-2643) "Investigating the Role of Proton Transfer of Porphyrin derivatives of Non-Linear Optics (NLO) Applications: DFT-Based Approach"
21. Neha Babar (2021-ag-2656) "DFT Study of Curcumin and its Derivatives for Zinc Scavenging"
22. Muhammad Asif (2021-ag-2681) "Improvement of Paper Strength with Borax Modified Starch"
23. Saliha Fatima (2021-ag-2682) "DFT Study of Pentacene Compounds for Efficient Linear and Nonlinear Optical Response Properties"
24. Rimsha Shareef (2021-ag-2687) "Novel Trimethoxybenzene-Based Dyes for Highly Efficient Dye-Sensitized Solar Cells"
25. Abaid Ullah (2021-ag-2592) "Benzodithiophene-Based Small Molecules for Organic Photovoltaic Applications"

#### Session: 2022-2024

1. Mubashra Laraib (2022-ag-1754) "A-D- $\pi$ -A- $\pi$ -D-A type diketopyrrolopyrrole based acceptors as efficient photovoltaic materials; A DFT approach"
2. Tania Shahzadi (2022-ag-1804) "Noncovalent interactions (NCI) analysis of non-fullerene solar cells acceptor materials by substituting end-capping groups"
3. Zara Fatima (2022-ag-1917) "Chitosan-graphene oxide composite as an effective adsorbent for the removal of dye from wastewater: DFT study"
4. Bakhtawar Ajaz Khan (2022-ag-1879) "DFT designation and investigation of Schiff-base derivatives"
5. Rimsha Naseem (2022-ag-1803) "DFT study of thermally activated delayed fluorescence (TADF) fluorescent materials"
6. Aqsa Laraib (2022-ag-1921) "Quantum study of Acyclovir drug: advanced oxidation pathways for STI application"
7. Asim Maqbool (2022-ag-1731) "DFT Study of natural antioxidants in Chinese tea"
8. Kainat Maryam (2022-ag-1940) "Theoretical investigation of NLO properties of DIBENZ [a,j] anthracenes based materials"
9. Gohar Iqbal (2022-ag-1752) "DFT study of Optoelectronic properties of acceptor materials for organic solar cells"
10. Maryam Rasheed (2022-ag-1908) "DFT study of advance oxidation process of acyclovir: STI applications"
11. Shehla Ashraf (2022-ag-1822) "Computational simulations of Schiff base materials"
12. Zunaira Saleem (2022-ag-1755) "Organic/Bio pesticides through density functional theory studies"
13. Muhammad Shahzad (2022-ag-1734) "Optoelectronic properties of Cyclopentadithiophene based donor-acceptor copolymers as donors., a DFT study"
14. Nazia Siddique (2022-ag-1738) "A DFT approach to study therapeutic potential of graphitic Carbon Nitride as a drug delivery material"
15. Hafiza Sana Saeed Rana (2022-ag-1907) "DFT analysis of natural dyes and pigments for food colouring"
16. Ramsha (2022-ag-1811) "Graphitic Carbon Nitride as a drug delivery system for anticancer drugs: A DFT approach"
17. Ayesha Farooq (2022-ag-1893) "DFT analysis of Schiff base molecules"
18. Noman Ali (2022-ag-1932) "DFT methods for drug designing: pharmaceutical applications"
19. Ghania Amjad (2022-ag-1753) "DFT Study of Pyrazine-fused carbene Au (I) based emitters for TADF materials"
20. Jannat Bibi (2022-ag-1826) "Quantum chemical properties of a pyrene substituted 1,3,4-oxadiazole derivatives properties"
21. Nimra Niaz (2022-ag-1805) "DFT analysis of biopesticides for promoting sustainable agriculture"
22. Shumaila Malik (2022-ag-2740) "Design of novel TADF materials for high efficiency organic light-emitting diodes (OLEDs)"
23. Syed Moman Ali Rizvi (2022-ag-2780) "TADF-based sensors and detectors: harnessing delayed fluorescence for sensing applications"

24. Uswa Mustafa (2022-ag-2744) "Enhanced nonlinear optical response through quantum chemical tailoring of boron and nitrogen-doped polyaromatic hydrocarbons"
25. Adan Ahmad (2022-ag-2785) "Quantum chemical study of phenyl based derivatives by utilizing DFT approach to investigate their NLO response"
26. Amina Faiz (2022-ag-2846) "Designing Novel Pazopanib Derivatives with Improved Specificity and Potency for Chronic Myelogenous Leukemia Treatment Using Structure-Based Computational Methods"
27. Ariha Zaid (2022-ag-2770) "Harnessing the pharmacological properties of Piperine analogues for dual inhibition of arthritis and antibiotic resistance"
28. Iqra Kaifi (2022-ag-2739) "A theoretical quantum chemical approach to explore large second hyperpolarizability and nonlinear optical response of [7]helicene derivatives employing DFT study"
29. Fajar (2022-ag-2775) "DFT Study of Graphene Oxide as a Potential Adsorbent for Hazardous Environmental Pollutants"
30. Syeda Sanam Zahra (2022-ag-2826) "Quantum chemical investigations of heterocyclic based dye-sensitized solar cell optical properties, and non-linear optical response"
31. Parsa Zainab (2022-ag-2793) "A DFT based modelling, spectroscopic characteristics and structure property relationships of triphenyl amine derivatives"
32. Maryam Zahra (2022-ag-2827) "First principal studies of the optical switching materials, structural modifications for higher nonlinear optical amplitudes"
33. Sonia Mukhtar (2022-ag-2878) "First principle studies of the hybrid iridium based photochromic complexes for the modulation of NLO response"
34. Khadija Ahmad (2022-ag-2753) "Multi-directional-electron acceptors for organic photovoltaics"
35. Sara Ashfaq (2022-ag-2845) "DFT studies on interaction of anticancer drug with nucleobases"
36. Khadija Azam (2022-ag-2902) "Metal complexes as TADF emitters: A computational study"
37. Misbah Basharat (2022-ag-2901) "Metal complexes as TADF emitters: a DFT study"
38. Farwa Batool (2022-ag-2800) "Interactions between  $\beta$ -cyclodextrin as a carrier for anti-cancer drug delivery"
39. Nimra Javed (2022-ag-2804) "DFT studies on interaction of anticancer drug with DNA"
40. Sana Qamar (2022-ag-2779) "DFT study to design efficient donors for organic solar cells"
41. Muhammad Huzaifa Mujeeb (2022-ag-2741) "Significant improvement of dye-sensitized solar cell performance using DFT methods"
42. Ayesha Rasool (2021-ag-2818) "Computational design of efficient non-fullerene acceptors for organic solar cells applications"
43. Muhammad Faisal Hasnain (2022-ag-2847) "Designing and theoretical characterization of small molecules for dye sensitized solar cells"
44. Bilal Mustafa (2022-ag-2809) "DFT study of pollutant dyes in wastewater"
45. Eman Jamil (2022-ag-2806) "Tuning of optoelectronic properties of solar cell acceptor molecules"
46. Asia Iqbal (2022-ag-2877) "DFT study of dye sensitized solar cells materials"
47. Zohra Munawar (2022-ag-2840) "Anticancer drug delivery system: A quantum chemical approach"
48. Muhammad Siddiq (2022-ag-2854) "Wastewater treatment for removal of toxic dyes; A DFT study"
49. Muhammad Umar Nadeem (2018-ag-3988) "DFT study of cyclopentadithiophene based copolymers for solar cells"
50. Mehboob Hassan (2022-ag-2896) "DFT analysis of drugs; Pharmaceuticals applications"
51. Muhammad Javid (2021-ag-2655) "DFT study of Schiff Base, Molecular structure and spectroscopic properties"
52. Amna Tahir (2022-ag-2771) "SERS platform for characterization of serum samples of colon cancer patients using silver nanoparticles as SERS substrate"
53. Sehar Nawabzadi (2020-ag-2879) "Surface-enhanced Raman Spectral characterization of blood serum samples of thyroid stimulating hormone (TSH) patients using 30 kDa"
54. Iqra Yaseen (2022-ag-2760) "SERS platform for characterization of serum samples of gallbladder cancer patients using silver nanoparticles as SERS substrate"

55. Mohammad Madni Atta (2022-ag-2792) "Surface-enhanced Raman Spectral characterization of different stages of germ cell tumor using serum samples of affected individuals"
56. Saira Dastgir (2022-ag-2768) "Surface-enhanced Raman Spectroscopy for the analysis of cell mass and supernatants of different bacterial strains"
57. Kaneez Fatima (2022-ag-2818) "Surface-enhanced Raman Spectral characterization of antibacterial activity of silver nanoparticles synthesized biological reduction method against Escherichia coli"
58. Saima Afzal (2022-ag-2880) "Surface-enhanced Raman Spectral characterization of serum samples of urinary bladder cancer patients of different stages"
59. Yousra (2022-ag-2769) "Surface-enhanced Raman Spectroscopy for the characterization of supernatants of biofilm forming Klebsiella Pneumoniae".
60. Faiza Nawaz (2022-ag-2862) "Extraction of phytochemicals from solanum Nigarium therapeutic potential: DFT molecular docking and analytical characterization"
61. Iqra Yasmeen (2022-ag-2783) "Extraction of phytochemicals from Millettia pinnata and their pharmacological potential".

#### Session: 2023-2025

1. **Sundas Farooq (2019-ag-5656)** "Molecular docking and computational studies of biologically important compounds for designing new drug molecules".
2. **Nimra Aamir (2023-ag-1129)** "Nonlinear optical study of organic compounds for optical applications".
3. Sadia Saddique (2023-ag-1138) "NLO stimulations for organic molecules using Density functional theory".
4. Irfa Areej (2023-ag-1203) "Designing nonlinear optical molecules by using computational methods".
5. Zainab Abid (2019-ag-5645) "Nanocarriers in Anticancer Drug Delivery: Insights from computational chemistry".
6. Nimra Jabbar (2019-ag-5668) "Computational Insights into Nanostructure-Based Drug Delivery Systems: A DFT Approach".
7. Danish Ali (2023-ag-1177) "Optoelectronic Investigation of small molecules donors for organic solar cell applications: A DFT study".
8. Maryam Maqbool (2023-ag-1197) "Thermally Activated Delayed Fluorescent Materials for Optoelectronic applications: A DFT study on TADF Emitters".
9. Hijab Gillani (2023-ag-1118) "Interactions between microplastics and pollutants in wastewater- A quantum mechanical approach".
10. Fazeeha Iman (2023-ag-1187) "Microplastics; as carriers of 3BHA: A study on adsorption and environmental impact".
11. Tahreem Fatima (2023-ag-1189) "DFT designation and investigation of Schiff-base molecules as pharmaceutical agents".
12. Hafsa Afzal (2023-ag-1218) "Exploring the Electronic and Pharmacological Potential of Schiff Bases Using Computational Approach".
13. Maria Saleem (2023-ag-1209) "Removing pollutants from wastewater by microplastics; A DFT study".
14. Laraib Jahan (2023-ag-1196) "Thermally activated delayed fluorescence (TADF): revolutionizing OLEDs for display and lighting applications".
15. Rida Fatima (2019-ag-5555) "DFT Approach For Designing Organic Nonlinear Optical Materials For Optoelectronic Devices".
16. Muneeb Ahmad (2023-ag-1793) "Molecular Engineering of Organic Nonlinear Optical Materials for Improved Second and Third Harmonic Generation".
17. Muhammad Husnain (2023-ag-1763) "Computational Approach in Drug Design: A Study on Molecular Docking and Virtual Screening".
18. Sehrish Ehsan (2023-ag-1791) "Quantum Chemical Approach to Investigate Nonlinear Optical Behavior in Organic Materials".
19. Wajeelha Asghar (2023-ag-1801) "Computational Exploration of Nlo Properties of Organic Derivatives Tuned by Structural Modification".
20. Hafiza Rayia Ramzan (2023-ag-1849) "Designation and Investigation of Organic Nonlinear Optical Materials for Their Applications in Optoelectronic Devices".
21. Hafsa Irshad (2019-ag-6695) "Computational Approach in Solar Cell: A Study on Donor-Based Molecules in Dye-Sensitized Solar Cell"
22. Sadia Ashraf (2023-ag-1780) "Charge Transfer and Binding Energies of Anticancer Drugs with Nanocages: Insights from DFT Studies".
23. Usama Ijaz (2023-ag-1821) "DFT Study to Design Efficient Small Molecular Dyes for OPVs",
24. Maria Ashfaq (2019-ag-5689) "Computational Study of Medicinal Plants Using DFT".
25. Tooba Farooq (2023-ag-1792) "Adsorption of Anticancer Drug on Doped and Functionalized Graphene; DFT Study".
26. Mubarra Iqbal (2023-ag-1786) Theoretical Investigation of Anticancer Drug Encapsulation in Nanocages: A DFT Study

27. Tehreem Saleemi (2023-ag-1847) "Computational Investigation of Anticancer Drug Delivery Materials".
28. Mehnaz kousar (2019-ag-3312) "DFT Study of Drugs Extracted from Medicinal Plants".
29. Abdul Hae Abid (2019-ag-5325) "Designation of High-Performance Dye-Sensitized Solar Cell Materials: Using DFT Methods".
30. Shifa Tehreem (2019-ag-5532) "Medicinal and Edible Plants: A Natural Source for Pharmaceutical Application".
31. Gulshan Jabeen (2023-ag-1804) "Exploring Pesticide-Graphene Oxide Interaction: Insights from Density Functional Theory".
32. Muqaddas Salam (2023-ag-1808) "Molecular Dynamics and DFT Studies on The Adsorption Efficiency of Selected Pesticides on Functionalized Graphene Oxide".
33. Waleejah Maqbool (2023-ag-1766) "DFT Study on Optoelectronic Properties of Novel Organic Dyes for Enhanced DSSc".

#### Session: 2024-2026

1. Faiza Luqman (2020-ag-5476) "Designing of Organic Chromophores with Enhanced Nonlinear Optical Properties"
2. Aqsa Ijaz (2020-ag-5480) "Computational Study of Drug Delivery Systems using Nano Carriers"
3. Rabia Arshad (2020-ag-5487) "DFT Analysis of hole Transport Materials for Perovskite Organic Solar Cell"
4. Tayyaba Batool (2020-ag-7075) "Design and Evaluation of Nanocarrier Systems using DFT for Optimized Drug Delivery"
5. Maida Amin (2020-ag-9405) "Design and Theoretical Analysis of Semiconductor Photocatalysts for efficient Water Splitting and Hydrogen Generation"
6. Rahat Asghar (2020-ag-9432) "Chemistry of Pesticide on Nano-Adsorbents via Density Functional Theory"
7. Ayesha Mehtab (2020-ag-9498) "Tailoring of Organic Semiconductor Materials for Enhanced Perovskite Solar Cells"
8. Irsa Zaib (2020-ag-9528) "Nanocarrier Design for Enhanced Drug Delivery Systems for Pharmaceutical Applications"
9. Sehar Fatima (2020-ag-9599) "DFT Study of High Performance Pesticides"
10. Lubna Ijaz (2024-ag-991) "A Computational and Theoretical Investigation of Non-Covalent Interactions in Molecular Systems"
11. Maryam Shabbir (2024-ag-993) "Theoretical Investigation of Single-Atom Catalysts for Enhanced Catalytic Performance"
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14. Hamna Nazir (2024-ag-1008) "Computational Insights into Small Donor Molecules for Organic Solar Cells Applications"

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Web of Science ResearcherID A6V-7893-2022

**January 3<sup>rd</sup> 2025 I. F=364.52**

**Total = 112 (First Author=17 Co-author=53 Corresponding author= 44)**

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#### CONFRENESS PAPER

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#### EVENTS ORGANIZED AS ORGANIZER

Organized 2<sup>nd</sup> "1Day *International Workshop on "Computational Techniques, AI and ReserchTools-2026* on July 22<sup>nd</sup>, 2025, at the New Senate Hall, UAF.

#### EVENTS ORGANIZED AS ORGANIZING SECRETARY

1. Organized Two days *1st International Symposium on "FRONTIERS IN COMPUTATIONAL CHEMISTRY (FCC-2022)"* at Department of Chemistry, University of Agriculture, Faisalabad, July 4-5th, 2022.
2. *Organized 1st International seminar on "DFT: A Multidimensional Exploration" (DFT-ME 2024)* on July 23<sup>rd</sup>, 2024, at the Science Block Lecture Theatre, UAF.
3. Organized 1st International Workshop on " One-Day International Workshop Entitled As "Advanced Modeling with Machine Learning & Computational Tools -2025 on 16<sup>th</sup> June 2025, at the IT building-CS Floor, UAF.

#### EVENTS ACTED AS ORGANIZING COMMITTEE MEMBER

4. Acted as **Organizing committee member** of "International Conference of chemistry, Materials and Technology (CMT-2023)" at Department of Chemistry, University of Agriculture, Faisalabad, March 15-16th, 2023.
5. **Acted as Organizing committee member of** "poster management/scientific/registration committee" International Conference on Functional Materials and Emerging Technologies (ICFMET-2024)" at Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
6. **Acted as Organizing committee member** publication in "two-day International Symposium" on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.

7. **Acted as Organizing committee member** in “One Day Nano-Tech Meeting on Wastewater Treatment” at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3rd, 2019.
8. **Acted as Organizing committee member** in ‘**National Workshop on Technical and Patent Writing**’ by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, January 28<sup>th</sup>, 2017.
9. Acted as Organizing committee member in ‘three-days International Conference’ on Role of Chemistry for Sustainable Development, jointly organized by GCUF, GCWUF & UAF, October 21-23, 2025.
10. Acted as **Organizing committee member** in two days’ Workshop on ‘use of essential Software in Academic Writing’ by community college, Department of Chemistry, University of Agriculture Faisalabad-Pakistan, 21-22<sup>nd</sup> December h, 2022.

### **TRAINING**

1. Participation in ‘*National training Workshop on X-ray Crystallography*’ by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, November 7-December 2, 2016.
2. Participation in a *two-day training workshop “Statistical Methods for Researchers using R”* by Department of Mathematics and Statistics, University of Agriculture Faisalabad-Pakistan, August 09-10, 2017. University Faisalabad, Pakistan, May 4 - 5, 2017.
3. Participation in ‘*National training Workshop on Advanced Spectroscopic techniques for Characterization of organic Compounds*’ by Department of Chemistry and Central Hi-Tech Laboratory, University of Agriculture Faisalabad-Pakistan, August 15-16, 2017.
4. Participation in *International training on “Recent Advances in Computational Chemistry” at Institute of Theoretical Chemistry, Jilin University Changchun 130023, China*, Under “One Road One Belt Project” (Grant # DL20180036) from State Administration of Foreign Expert Affairs of China Aug. 08-21, 2019.
5. *Participated in two days Election Training of presiding officer* at Government Crescent School, Faisalabad, arranged *by Election Commission of Pakistan*, in May 2023.
6. *Participated in two days Election Training of presiding officer* at Faisalabad, arranged *by Election Commission of Pakistan*, in May 2018.
7. **Participated in in Training workshop for National Agriculture** education accreditation council (NAEAC) Program evaluators, organized by NAEAC council, Islamabad Pakistan, in Jan 1<sup>st</sup>, 2024.
8. Participation in “*International Workshop on Capacity Building of National Scientist and relevant Stakeholders on “Agriculture Policy”*” at CAS, University of Agriculture Faisalabad, Pakistan, 19th May to 13th June 2025.
9. Participation in “*Two Days HPC User-Level training*” at IT, University of Agriculture Faisalabad, Pakistan, 26-27th May to 13th June 2025.
10. Participation in “*Two Day Hands-On Training Workshop* on Patents and Funded Projects for Profitable Research with Industries “at Government College for Women University Faisalabad, 18-19 August 2025.
11. Participation in “Online Training session” as conveyor of departmental Program Review Effectiveness and Enhancement (PREE) committee organized by QEC-UAF at 2:30pm on December 12th , 2025.

12. Participated a Professional Development Session on “**Paper Setting, Evaluation, and Result Submission**” for **Secretaries of Faculty Board and Focal Persons of OBE** on 05 May 2026 at DLC-II, Faculty of Agriculture-UAF organized by Director Academics.
13. Acted as committee member of committee for **Short Skill Development Course Training “Atomic spectroscopic techniques”** on 12-15th May 2026 at department of Chemistry, University of Agriculture Faisalabad.
14. Participation in “**Training session**” as conveyor of departmental Program Review Effectiveness and Enhancement (PRE) committee organized by QEC-UAF at NIFSAT -UAF on May 13th, 2026.
15. Online participation in International training entitled “Water Governance and IWRM: Principles, Practices and Tools” Jointly organized by COMSTECH, SUEN & GD of Water Management (Turkiye)” organized by OIC – COMSTECH 9 & 10 June 2026 (12:00 PM – 04:00 PM, Pakistan time (Join Zoom Meeting<https://us02web.zoom.us/j/83462421973?pwd=QY1oCPpSmOJ1b0UDI2K5viY9UOZCfb.1>)).
16. Participation in “**3-Day Training Workshop for Senior Faculty at University of Agriculture**, Faisalabad (UAF) organized by Director orate of academics UAF from July 14th-16th , 2026.
17. Participation in “**Training Workshop on Capacity Building of UAF Faculty for Artificial-Intelligence-Basics & Applications**” organized by Department of Computer Science, UAF from 13th – 22nd July , 2026
18. Participation in “Online **TRAINING SESSIONS ON CURRICULUM REVIEW – 31 JULY 2026**” organized by Directorate Academics-UAF.

#### **Acted as member of Tender Purchase committee**

- a. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as “Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops”.
- b. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as “Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops”, held on February 3<sup>rd</sup>, 2022.
- c. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as “Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops”, held on February 9<sup>th</sup>, 2022.

#### **ORAL /POSTER PRESENTATIONS**

19. **Abstract publication and Oral Presentation** in ‘7<sup>th</sup> International Conference “Environmentally Sustainable Development”, ESDev-2017’ at CIIT Abbottabad, Pakistan, August 26-28, 2017.
20. **Oral Presentation and Abstract publication** in ‘2<sup>nd</sup> international conference Chemistry Conference of Biochemistry, Biotechnology and Biomaterials, 2018 at Department of Biochemistry, University of Agriculture, Faisalabad, Pakistan, December 09-011, 2018.
21. **Poster Presentation and Abstract publication** in ‘two-day International Symposium’ on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.
22. **Poster presentation and abstract publication** in “2<sup>nd</sup> International Conference on Recent Advances in Chemical Sciences, ICRAC 2019” at Department of Chemistry, GC University Lahore, Mar 20-22, 2019.
23. **Oral Presentation and Abstract publication** in ‘International Chemistry Conference forefronts of Chemistry, Celebrating the Periodic Table Year’, at Institute of Chemical Sciences BZU Multan, Mar 27-29, 2019.

24. **Oral Presentation and Abstract** publication in ‘The Seventeenth International Symposium on Electroanalytical Chemistry & The Third International Meeting on Electrogenated Chemiluminescence (17th ISEAC & 3rd ECL)’, at Changchun Institute of Applied Chemistry Chinese Academy of Sciences 5625 Renmin Street, Changchun, Jilin 130022, China, Aug 22-25, 2019.
25. **Invited speaker in “Multidisciplinary Approach towards Computational Chemistry”**, at GCWUF, Faisalabad, Sep 25-26, 2019.
26. **Oral presentation as Invited speaker** in “2<sup>nd</sup> International Conference on Advances in Theoretical and Applied Physics”, at GCWUF, Faisalabad, Mar 2-3, 2020.
27. **Oral presentation as Guest speaker** in “International Conference on Advances in Experimental and Theoretical Physics”, at UAF, Faisalabad, Mar 4-5, 2020.
28. **Oral Presentation** in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28<sup>th</sup>, 2022.
29. **Poster Presentation** in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28<sup>th</sup>, 2022.
30. **Oral Presentation** in Two Day 5<sup>th</sup> National and 1<sup>st</sup> International Symposium on Writing Science and Leveraging Scientific Research, organized by Department of Chemistry, University of Agriculture, Faisalabad, March 02-03, 2022.
31. **Oral Presentation** in workshop on “Helping People to Develop safe and Sustainable Water for Use”, organized by Department of Chemistry, University of Agriculture, Faisalabad, December 23<sup>rd</sup>, 2022.
32. **Oral Presentation** in online webinar on “Molecular Docking and DFT studies for Drugs Development” organized by Department of Chemistry, University of Agriculture Faisalabad Pakistan, on 25<sup>th</sup> January.
33. **Invited Talk** in Three Days 4<sup>th</sup> International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, December 4-6<sup>th</sup>, 2024.
34. **Invited Talk** in Three Days International Conference on “Natural Products: Biological and pharmaceutical Applications”, organized by Department of Chemistry, Government College Women University, Faisalabad, December 18-20<sup>th</sup>, 2024.
35. **Invited Talk** as Keynote speaker in One day International Symposium on “1<sup>st</sup> International Symposium on Computational Chemistry/Machine Learning”, organized by Department of Chemistry, COMSATS University Islamabad, Lahore Campus, April 16, 2025.
36. **Oral Presentation** in Two Day Seminar on “Scientific Writing with LATEX”, organized by UAF Community College, Department of Chemistry, University of Agriculture, Faisalabad, May 05-06, 2026.

#### **PARTICIPATION IN CONFERENCES/WORKSHOPS/ REFRESHER COURSES & TRAININGS**

37. **18th National Chemistry Conference, Institute of Chemistry, University of the Punjab, Lahore**, Chemical Society of Pakistan, Feb. 2008.
38. **International Conference** on Computational Chemistry and Biology (ICCCB) November 2012 Shenzhen, China.
39. **International Conference** on Theoretical and High Performance Computational Chemistry 2012, Nanjing, China
40. The Seventh International Conference on Theoretical Chemistry Molecular Modeling and Life Sciences as well as Academic Intercommunion on the Platform for Scientific Computation and Simulation Software (7th ICTCLS), Beijing, China, July 2013.
41. The **12th National Conference** of Quantum Chemistry (NCQC), Taiyuan, China, June 2014.

42. Participation in '**National Grant Writing Workshop**' by US-Pakistan center for Advance Studies in Agriculture and Food Security (USPCAS-AFS) at UAF, April 6-7, 2016.
43. Participation in **National workshop** on "Organic Food and Health: Avenues of Innovation and entrepreneurship" University of Management and technology, Lahore, Pakistan by Pakistan Council for Science and Technology (PCST), August 29, 2016.
44. Participation in '**International Conference** on Energy for Environmental and Economic Sustainability (ICEEES2016)' Lahore, Pakistan October 20 - 23, 2016.
45. Participation in '27th National and **International Chemistry Conference** at Department of Chemistry', University of Malakand, Khyber Pakhtunkhwa, Pakistan. August 22-25, 2016.
46. Participation in '**National Symposium on Emerging Trends in Applied Physics**' by Department of Physics, University of Agriculture Faisalabad-Pakistan, December 3, 2016.
47. Participation in '**National Workshop on Technical and Patent Writing**' by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, January 28<sup>th</sup>, 2017.
48. Participation in '**National Seminar on FT-IR and FT-NIR Applications**' by Rays Technologies (Bruker) Lahore-Pakistan, February 14, 2017.
49. Participation in "6<sup>th</sup> **Technical Workshop on Statistical Analysis**" by Department of Chemistry, University of Sargodha, Women Campus Faisalabad-Pakistan, May 06, 2017.
50. **Participation, abstract publication in '10<sup>th</sup> Chemistry Conference 2018 "Chemistry in Engineering and Life Sciences", at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.**
51. **Participation in " International Conference on Modern Trends in Chemistry and Energy Technologies" Departments of Chemistry, Pharmacy and Energy Research Center, COMSATS University Islamabad, Lahore Campus-Pakistan, October 22-23 2018.**
52. **Research collaboration visit to "Institute of Theoretical Chemistry, Jilin University, Changchun, PR China Under "One Road One Belt Project" " (Grant # DL20180036) from November 23-30<sup>th</sup>, 2018 from State Administration of Foreign Expert Affairs of China and collaboration bond was signed between "Institute of Theoretical Chemistry, Jilin University and Department of Chemistry, University of Agriculture, Faisalabad, Pakistan.**
53. **Participation in '2<sup>nd</sup> international Symposium on Pharmaceutical Sciences at GC University Faisalabad, Pakistan, January 30<sup>th</sup>, 2019.**
54. **Participation in 'two day International Symposium" on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.**
55. **Participation in "1<sup>st</sup> international Conference on Surface Sciences Innovations and Applications for Geoenviromental Challenges" at Institute of Soil and Environmental Sciences, University of Agriculture Faisalabad, Pakistan, April 25-26, 2019.**
56. **Participation in "One Day Nano-Tech Meeting on Wastewater Treatment" at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3<sup>rd</sup>, 2019.**
57. **Participation in "Two Days training GCWU May 2019.**
58. **Participation in "One Day Workshop on Fundamentals of Laboratory Biosafety" at Department of Biochemistry, University of Agriculture Faisalabad, Pakistan, Feb 24, 2020.**

59. Participation in “One Day 3<sup>rd</sup> National Symposium on One Health” at Faculty of Veterinary Sciences, University of Agriculture Faisalabad, Pakistan, Sep 8th, 2021.
60. Participation in “One Day Workshop on Discovering the innovative progressions in catalysis” at Faculty of Sciences, University of Agriculture Faisalabad, Pakistan, Dec 20th, 2021.
61. Participation in “Two Days 1<sup>st</sup> International Conference on Innovation in Chemistry & Physics at, Department of Chemistry and Physics, University of Education, Faisalabad Campus, Pakistan, March 14-15th, 2022.
62. **Participation** in “International Workshop on Capacity Building of national Scientist and relevant Stakeholders on MRL & Biopesticides” at Department of Entomology, University of Agriculture Faisalabad, Pakistan, Feb 16th, 2023.
63. Participation in one day seminar on “the use of essential oils and their nano formulations as alternatives of antibiotics and chemical for infection control and bio preservation” at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, Dec. 22nd, 2025.
64. Participation in one day seminar on “Electrochemical Energy Conversion and Storage” at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 11<sup>th</sup>, 2026.

#### **ONLINE PARTICIPATION IN DIFFERENT SCIENTIFIC ACTIVITIES**

1. **Participation in the National Artificial Intelligence Forum** organized by Sino-Pak Center for Artificial Intelligence (SPCAI), PAF-IASST, Haripur, Pakistan, on 2<sup>nd</sup> September 2021.
2. **Participation in a webinar (via Zoom)** on “Women in Science and Global Health” organized by Department of Pediatrics and Child Health, Aga Khan University, Karachi, Pakistan, on 25<sup>th</sup> November 2020.
3. **Participation in a webinar (via Zoom)** on “Capacity building for launching and Running a Successful Journal” organized by Department of Chemistry, GCWUF on 3rd December 2020.
4. **Participation in a webinar (via Zoom)** on ‘Management of Drinking Water, Dams, and Lake Basins Depending on The Changing Climate’ by COMSTECH - March 13, 2025.
5. **Online Participation in “OIC-COMSTECH and Ningbo University Certificate Course on Applied Biomedical AI” July-August 2025.**
6. Participation in “COMSTECH-HEALTHRAB JOINT WORKSHOP ON CLINICAL RESEARCH IN RESOURCE CONSTRAINED ENVIRONMENT” September 30<sup>th</sup>, 2025, 12PST.

#### **ABSTRACT PUBLISHED IN CONFERENCES**

1. **Abstract Published Shamsa Bibi, Shafiq-Ur-Rehman and JingPing Zhang**, “Theoretical Studies to Investigate the Effect of Different Cores in Two Different Topologies in Donor Materials toward Organic Solar Cells”. *Poster and abstract Published in “7th International Conference: Environmentally Sustainable Development – ESDev-VII” August 26-28<sup>th</sup> 2017.*
2. **Abstract publication in ‘10th Chemistry Conference 2018 “Chemistry in Engineering and Life Sciences”, at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.**
3. **Abstract publication**, entitled as “Gemcitabine-Based Anticancer Drug with Metal-Doped BN24 as a Drug Delivery Carrier: Density Functional Theory”, in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
4. **Abstract publication**, entitled as “Novel Phenolic Compounds as Potential Therapeutic Candidates Against SARS-Cov-2, Using Quantum Chemistry, Molecular Docking and Dynamic Studies: in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.

5. **Won 3rd Prize & Abstract publication**, entitled as “Novel Phenolic Compounds as Potential Therapeutic Candidates Against SARS-Cov-2, Using Quantum Chemistry, Molecular Docking and Dynamic Studies: in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
6. **Abstract publication**, entitled as “Fragmentation Mechanisms Of Secnidazole By Advanced Oxidation Processes: DFT Study”, in Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
7. **Abstract publication**, entitled as “Adsorption And Removal Of Manganese And Vanadium From Wastewater By Graphene Oxide /Chitosan Composites; A Computational Study”, in Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
8. **Abstract publication**, entitled as “A DFT Study Of Solvent Impact On The Photochemical Properties Of Anticancer Drugs PLX4720”, In Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
9. **Abstract publication**, entitled “*Innovative Computational Approaches for Designing Advanced Optoelectronics Materials towards Energy Applications*”, in the 4th International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by the Department of Chemistry, Government College Women University, Faisalabad, December 4-6th, 2024.
10. **Abstract publication**, entitled “*Computational Analysis of Ribofuranose Nucleoside Derivatives: Targeting EGFR and VEGFR2 in Cancer Cells*”, in the 4th International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by the Department of Chemistry, Government College Women University, Faisalabad, December 4-6th, 2024
11. **Won 3<sup>rd</sup> prize in poster & Abstract publication**, entitled “*Modeling 3Bha Adsorption on Polyethylene and Polypropylene Microplastics*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
12. **Abstract publication**, entitled “*Exploring Symmetry in Curcuminoids Derivatives for Performance of Photovoltaic Materials*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
13. **Abstract publication**, entitled “*Exploring the Anticancer Potential of Ribofuranose Nucleosides: A Combined DFT and Docking Study*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
14. **Abstract publication**, entitled “*Designing the Electron Push-Pull Chromophores for Efficient Nonlinear Optical And Photovoltaic Properties*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
15. **Abstract publication**, entitled “*Computational Studies of Phenothiazine-Based Derivatives for Fluorescent Applications in Semiconductors*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
16. **Abstract publication**, entitled “*Multicomponent Composite for Dye Remediation: Cellulose, Clay, and Sodium Alginate - A Combined Experimental and DFT Investigation*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
17. **Abstract publication**, entitled “*The Impact of Nanostructures on Targeted Drug Delivery of Anticancer Drugs using DFT Studies*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.

18. **Abstract publication**, entitled “*Optimizing Optoelectronic Properties of Quinoidal Oligomers Through Shape, Size, and Heteroatom Substitution*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
19. **Abstract publication**, entitled “*Quantum Chemical Approaches for Designing High-Performance Ladder-Shaped NLO Molecules*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
20. **Abstract publication**, entitled “*Superalkali  $X_3O$  ( $X = Li, Na, K$ ) Doped  $B_{12}N_{12}$  Nano-Cages as a New Drug Delivery Platform for Chloromethine: A DFT Approach*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
21. **Abstract publication**, entitled “*Computational Study of  $BC_3$  Graphene Interaction with Amantadine for Sensing Applications*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
22. **Abstract publication**, entitled “*Twisted Small Molecule Donors with Enhanced Intermolecular Interactions Towards Efficient all Small-Molecule Organic Solar Cells*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.

**The End**